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MICROSTRUCTURE MODELING OF THE SUPERALLOY INGOT BREAKDOWN PROCESS (PREPRINT)

Alexander R. Bandar, Ravi Shankar, Li Cai, and Wei-Tsu Wu

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14. ABSTRACT
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MICROSTRUCTURE MODELING OF THE SUPERALLOY INGOT BREAKDOWN PROCESS

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Keywords: Microstructure Modeling, Finite Element Modeling, Nickel Superalloy

Abstract

A microstructure evolution model is presented, integrated into the Finite Element Modeling (FEM) software package DEFORM™. Recrystallization and grain growth, during and after thermomechanical deformation, are predicted via a phenomenologically-informed Cellular Automata (CA) algorithm. Strain, strain rate, and temperature are computed via FEM and provided as inputs to the model. Examples of a CA technique to predict microstructure evolution during cogging of a nickel base superalloy are presented. Although this model is focused on and will be validated for cogging of nickel base superalloy U720, it is designed to accommodate a range of alloys, thermomechanical processes, and other microstructure evolution algorithms, such as Monte Carlo (MC) and Phase Field (PF) methods as well.

Introduction

Nickel base superalloys have excellent high-temperature creep and corrosion resistance, and are widely used in industry for turbine discs and blades. They are also expensive and often difficult to form[1]. U720 in particular, for which this research development was inspired, is a precipitation-hardened alloy, strengthened with a high volume (~40%) of phase $Ni_3(Al,Ti)$, with a solvus temperature of ~1153^o C. It has a narrow hot-working window, and is particularly susceptible to cracking during forming.

Large ingots of U720 are often cogged to more practical billet sizes for further forming. The cogging process is a metal forming technique whereby a short, wide ingot is reshaped into a long, narrower workpiece by the action of many repetitive die blows (Figure 1). This technique is useful not only for producing more practical workpiece geometries, but is also a necessary method to convert the large, non-uniform grains and chemical inhomogeneities present in a cast ingot into a more refined, uniform microstructure. This process of "ingot breakdown" is effective, though determining the optimum parameters –

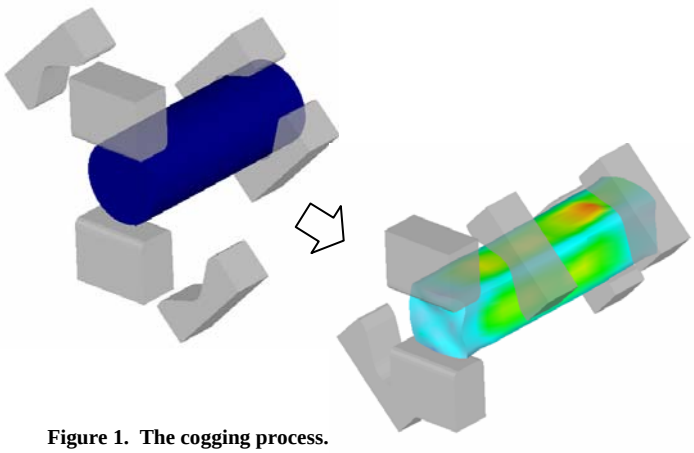


Figure 1. The cogging process.

the preheat, the number of die blows, the bite of each die, the rotation of the workpiece from pass to pass, etc., can be difficult. FEM software programs can provide manufacturers with a useful tool to optimize the thermomechanical parameters by simulating the process prior to executing it. It is additionally desirable to optimize the final microstructure, for which a practical microstructure evolution model, in addition to a practical FEM software package, is advantageous.

Microstructural evolution of nickel base superalloys, during and after cogging, may involve a wide variety of phenomena, occurring simultaneously or sequentially: grain shape change due to material flow, work hardening, dynamic recovery, dynamic recrystallization, metadynamic recrystallization, static recrystallization, static recovery, phase transformation, precipitation, and grain growth. In order to develop an efficient method to model this ingot breakdown process, Scientific Forming Technologies Corporation has engaged in numerous internally and externally funded research projects in conjunction with the United States Air Force and industrial partners. Recently SFTC was awarded a two-phase, three year SBIR grant from the USAF to further develop a microstructure model integrated into the commercial Finite Element Modeling code DEFORM^{TM}. Phase I, which was performed over one year, involved a literature survey of existing microstructure evolution models, preliminary development of such a model, preliminary investigation of Inverse Analysis to determine microstructure modeling materials constants, and other studies. Phase II, which will occur over the course of the next two years, will involve further development of this model, as well as validation of the results with laboratory and industrial scale experiments. The results presented in this paper represent the intermediate stage of development after Phase I and before Phase II, as well as internal development efforts on behalf of SFTC.

Microstructure Evolution – the JMAK Model

During deformation and heat treatment of a material, various microstructural phenomena can occur.–Different empirical, phenomenological, and first-principle models exist to predict the behavior of these phenomena over a variety of conditions. Each has their advantages and disadvantages. In the case of recrystallization, the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation has been the classical method of the last 70 years to compute average final grain sizes based on an initial average grain size, thermomechanical inputs, and various materials parameters[2].

$$X = 1 - \exp(-B\varepsilon^n) \qquad (1a)$$

$$X = 1 - \exp(-Bt^n) \qquad (1b)$$

In the JMAK model, newly recrystallized regions nucleate throughout a deformed microstructure at a certain rate (specified by the Avrami coefficient, *n*), and these regions grow and consume the microstructure at a certain speed (specified by the growth constant, *B*), consuming the stored energy (quantified in the form of a dislocation density) and ultimately impinging on the boundaries of other growing, recrystallizing regions. In the case of dynamic recrystallization, this is often modeled as a function of strain (Eq. 1a) – as energy is input into the material (in the form increasing dislocation density due to Frank-Read sources, Orowan looping, and other mechanisms), a threshold of energy will be reached and portions of the material will recrystallize. In the case of metadynamic or static recrystallization, JMAK modeling is typically computed as a function of time (Eq. 1b), indicative of the statistical necessity to wait for a probability of nucleation events to occur, and to permit those newly nucleated regions to grow.

To determine the values of *B* and *n*, sufficient material testing must be performed to characterize the microstructural response over the range of thermo-mechanical processing parameters (e.g.

strain, strain rate, and temperature) which bracket the range experienced during forming and heat treatment. The resultant test samples are then metallographically observed, and the fraction of recrystallization and the final grain sizes are quantified. For the range of strains, strain rates, and temperatures tested, the thermo-mechanical space is populated with the measured datapoints corresponding to the final microstructure (e.g. fraction recrystallized as a function of strain at a given temperature and strain rate). Then the JMAK equation is "curve-fitted" to match the experimental data. This technique is computationally efficient and can be reasonably accurate, provided that the stored energy in the material is uniformly distributed, that the recrystallizing phases grow isotropically, and that no non-linear events occur during recrystallization, such as formation of precipitates which, if small, may impede grain growth via Zener pinning; or, if large, may induce Particle Stimulated Nucleation (PSN. However, even if the material is not generally isotropic (e.g., in highly crystallographically textured alloys) there are methods to adjust for this – by varying the values of B and n with respect to time, for example. Even PSN can be accommodated for by further tweaking the JMAK parameters; but eventually a point will be reached where it is too cumbersome to continue adjusting these few variables to meet realistic experimental results, and it is simply more efficient to simulate a microstructure, and to model nucleation, growth, and other phenomena explicitly.

For example, in the ingot breakdown process, a point on the workpiece can undergo repetitive forming and heat transfer cycles. This is difficult to model exclusively using the JMAK technique, for the reasons given above. Additional difficult JMAK modeling challenges are:

- determining the dominant kinetics for recrystallization
- the large amount of material testing to characterize the model coefficients
- designing testing conditions to match the actual cogging process
- ambiguity in modeling the start-and-stop forming (dynamic recrystallization) and heat treatment (metal dynamic and static recrystallization) operation cycles

This is particularly the case for large cast ingots of nickel base superalloys, which tend to have a variation not only in grain size but in grain shape as well (due in part to directional thermal gradients during cooling). JMAK models are typically not sensitive to these different grain morphologies. In other words, microstructures of the same statistically average grain size but different grain shapes (for example, equiaxed vs. elongated grains) would be predicted to have the same microstructure evolution kinetics, which in reality is not the case (elongated grains have a higher grain boundary surface area, resulting in greater nucleation sites; additionally, they are narrower, resulting in through-grain impingement occurring sooner). Additionally, certain neighbor-to-neighbor grain boundary hot-spots may exist which locally deviate from average grain boundary behavior (resulting in abnormal grain growth, for example) These, and other coupled phenomena, are difficult to capture via JMAK alone. Thus, traditional JMAK modeling may not accurately predict the appropriate microstructure kinetics during ingot breakdown. Rather, a more holistic approach to microstructure evolution, which incorporates new, spatially-sensitive "Discrete Lattice" models, have been developed. Figure 2 depicts

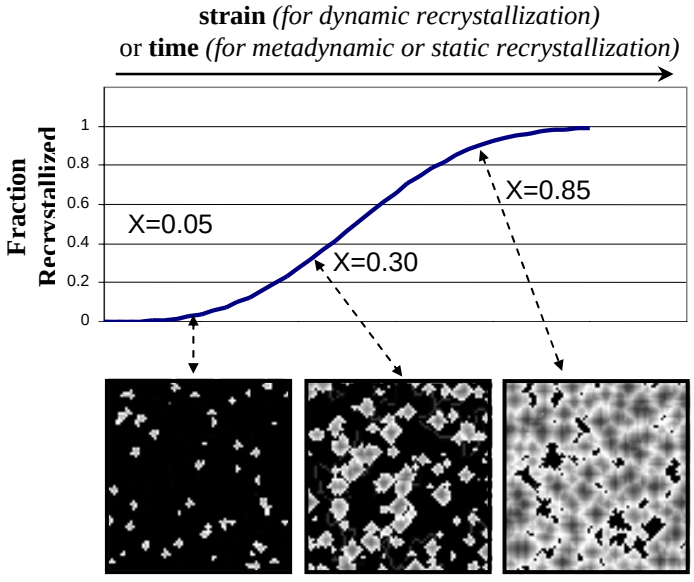


Figure 2. ***(Top)*** **Recrystallization kinetics computed by classical JMAK modeling.** ***(Bottom)*** **Recrystallization explicitly computed via Discrete Lattice modeling; (dark regions = deformed material; lighter regions = recrystallized material).**

the classical JMAK curve of recrystallization kinetics, as well as examples of equivalent Discrete Lattice recrystallization modeling, below.

Microstructure Evolution – the Discrete Lattice Model

Discrete Lattice models represent a microstructure as a discrete lattice of regularly arrayed points, for which each point is representative of a microstructure feature, such as crystallographic orientation, dislocation density, chemical concentrations, etc. Such a model, which represents grains and grain boundaries explicitly (rather than as an "average" value), *is* sensitive to local variations in grain geometry, and as such, can more appropriately capture the behavior of neighbor-to-neighbor reactions (recrystallization, for example) than classical JMAK models.

To capture the various microstructure evolution phenomena, as well as to develop a model sensitive to the different initial grain morphologies present in a cast ingot, various Discrete Lattice neighbor-to-neighbor-sensitive microstructure evolution algorithms were investigated. These included Cellular Automata (CA), Monte Carlo (MC), and Phase Field (PF) techniques[3,4,5]. Ultimately, the CA technique was selected for its optimum combination of computational efficiency and the accuracy of modeling microstructural phenomena relevant to metal forming and heat treatment processes.

Discrete Lattice Modeling Methodology

Currently, the microstructure evolution model presented is uncoupled to FEM calculations. That is, an FEM simulation is first performed, and the thermomechanical histories (strain, strain rate, temperature) of one or more points on the workpiece are computed at each time step. These values are then provided as thermomechanical inputs to the microstructure evolution module. An initial microstructure, with statistics similar to the real microstructure to be modeled, is generated, on which is then computed work hardening, recovery, recrystallization, and grain growth throughout the forming and/or heat treatment processes.

The initial microstructure represented by the CA is created with a given height (H) and width (W) in cells, a given ratio of microns to cell, and an initial average grain diameter (D) to generate. The area of the simulated region is divided by the average grain area to determine the starting number of grain nuclei (N_i) necessary to initialize the microstructure.

$$N_i = \left(H \cdot W\right)\left(\mu m / cell\right)^2 \Big/ \pi\left(D/2\right)^2 \qquad (2)$$

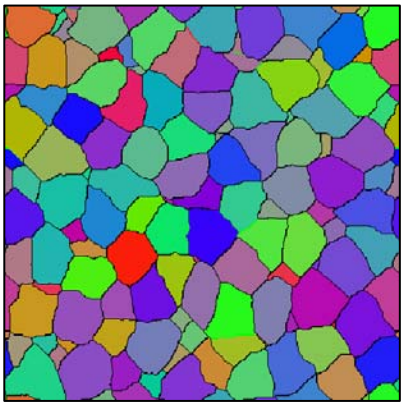


Figure 3. Example initial microstructure. Colors represeent different crystallographic orientations.

Random (x,y) coordinates throughout the CA are then chosen for each nucleus; a random crystallographic orientation (defined in terms of Euler angles ϕ_1, Φ, ϕ_2) is associated with that nucleus, and the nuclei are allowed to grow to impingement, via the traditional CA algorithm. (That is to say, if neighbor cells of a nucleus are not part of a grain yet, then those neighbors adopt the crystallographic orientation of the cell; repeat until no unvisited cells exist) The CA model is presently a square 2D grid; Moore's neighborhood is used (only neighbors, and not neighbors of neighbors, transform each time step), and it is periodically bounded on all sides. Once all cells have been transformed, the grains and hence grain boundaries of the microstructure have been determined. A starting value for the dislocation density of each cell is initialized (e.g. 0.01 $\mu m/\mu m^2$, for a typical annealed metal[6]). At this point, the microstructure is ready for evolution.

Presently, four microstructural phenomena are modeled: work hardening, recovery, recrystallization, and grain growth. Within the phenomenon of recrystallization, 3 types are separately modeled: dynamic, metadynamic, and static. It should be noted that the same method can be used for precipitation and phase transformation, although they are not included in the current implementation.

To begin, one or more regions of interest on the workpiece are selected, and simulated microstructures are initialized for each. Then, for each microstructure, the following cycle is computed every time step:

- FEM point-tracking of the strain, strain rate, and temperature of each region of interest on the workpiece is provided to the microstructure model
  - the dislocation density for each cell in the microstructure is updated as a function of these inputs and of the current dislocation density (i.e. work hardening and recovery)
  - the energy of the microstructure is evaluated at each cell, and high-energy regions (such as triple points and grain boundaries, with energies given by Read-Shockley) are identified
  - if the dislocation density at any high-energy regions exceeds a critical value, then a recrystallization nucleus is spawned there: a grain of a single cell with a new, random set of Euler angles (resulting in high-angle boundaries with neighboring grains) is placed at the critical, high-energy point, and the dislocation density is reset to a recrystallized (e.g. annealed) value
  - any previously existing recrystallized grains advance through the surrounding work-hardened material; they stop when they impinge at recrystallized boundaries
  - grain growth is performed, where grain boundary velocities are functions of temperature and misorientation (calculable from the two sets of Euler angles of the grains on either side of the boundary)

Work hardening and recovery are computed via a modified Laasraoui-Jonas equation[6], (Eq. 3), and tracked at each cell within the Discrete Lattice as a dislocation density value.

$$d\rho_i = \left(h - r\rho_i\right) d\varepsilon \qquad (3)$$

The Laasraoui-Jonas equation is a hardening and recovery model, where $d\rho_i$ is the change in dislocation density due to a hardening term *(h)* and a recovery term *(r)* for a particular cell, given below; ρ_i is the instantaneous dislocation density for the cell; $d\varepsilon$ is the increment of strain, when deforming; (this is replaced with time, *dt*, if heat treating).

$$h = h_0 \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)^m \exp\left(\frac{mQ}{RT} \right) \qquad (4)$$

$$r = r_0 \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)^{-m} \exp\left(\frac{-mQ}{RT} \right) \qquad (5)$$

$\dot{\varepsilon}$ is the strain rate at the point being tracked; T is the temperature; Q is an activation energy; R is the gas constant, and h_0, $\dot{\varepsilon}_0$, and m are materials constants[6].

Thus, as strain ($d\varepsilon$) increases, a change in the dislocation density is computed at each discrete lattice point, which is the difference between the portion added due to hardening ($hd\varepsilon$), and the difference removed due to recovery ($-r\rho_i d\varepsilon$). The recovery term is deducted from certain cells selected in the CA via a stochastic manner as described by R. Goetz[3]. Examples of these phenomena are displayed in Figures 4 and 5.

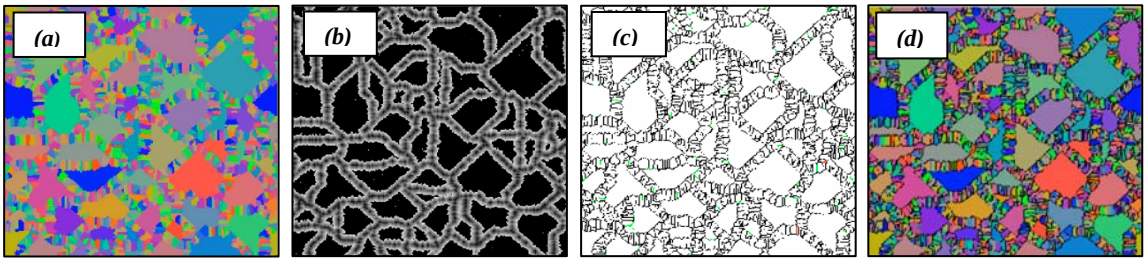


Figure 4. (a) oiginal and recrystallizing grains, color-coded by crystallographic orientation; (b) dislocation density map; dark = high dislocation density (deformed material); light = low (recrystallized material); (c) grain boundary map, used to determine high-energy regions for nucleation sites; black = high angle boundary ($\theta > 15^o$); green = medium angle ($15^o > \theta > 5^o$); red = low angle ($\theta < 5^o$). (d) composite map of grain orientations and grain boundary misorientations.

Presently, grain growth is performed by assigning velocities to grain boundaries as functions of temperature and/or of crystallographic misorientation, but will ultimately be driven by grain boundary curvature as well (since curvature is a locally-calculable feature of a Discrete Lattice representation – one of the motivations for selecting this type of data structure). Grain boundary velocities can be related to grain boundary energies defined by Read-Shockley, as explained above, or by more complicated grain boundary energy functions of misorientation, which include pinning at coincident site lattices and other low-energy orientations, which can give rise to texture effects during recrystallization.

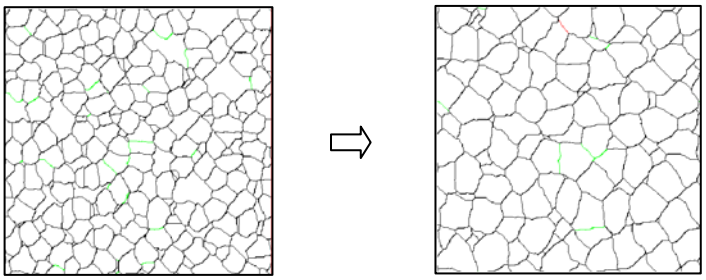


Figure 5. Depiction of grain growth. Grain boundary velocities are functions of temperature and misorientation; misorientations are color-coded: black = high angle boundary ($\theta > 15^o$); green = medium angle ($15^o > \theta > 5^o$); red = low angle ($\theta < 5^o$).

Comparison of JMAK Modeling to Discrete Lattice Modeling

Comparison of the kinetics of dynamic recrystallization, as predicted by the classical JMAK model, and as predicted by the new Discrete Lattice model, are presented in Figures 6 and 7. A double-cone compression test was simulated and three regions of interest "point-tracked" (Figure 6, top left). The thermomechanical values at the three locations were exported (Figure 6, top right) as inputs to the microstructure model. The microstructure model then calculated work hardening, recovery, recrystallization, and grain growth for every time step; recrystallization maps at 0%, 30%, and 60% compression are presented (Figure 6, bottom left). The fractions recrystallized for each region of interest were plotted as a function of compression of the double-cone test specimen, and compared with classical JMAK modeling predictions (Figure 7). The comparison is qualitatively and quantitatively similar.

Discrete Lattice Modeling : Sensitivity to Microstructure Morphology

Due to the fact that a Discrete Lattice algorithm models the spatial representation of grains, grain boundaries, phases, etc., the microstructure evolution kinetics are sensitive to grain boundary shapes. This is not true of the classical JMAK modeling method. Since real microstructures often exhibit non-equiaxed grains (e.g. ingots with cast microstructures, pre-form parts with wrought microstructures from previous deformation, or heat-treated parts where grains may have grown non-uniformly due to temperature gradients, etc.), this represents an improvement in the accuracy of realistic microstructure modeling.

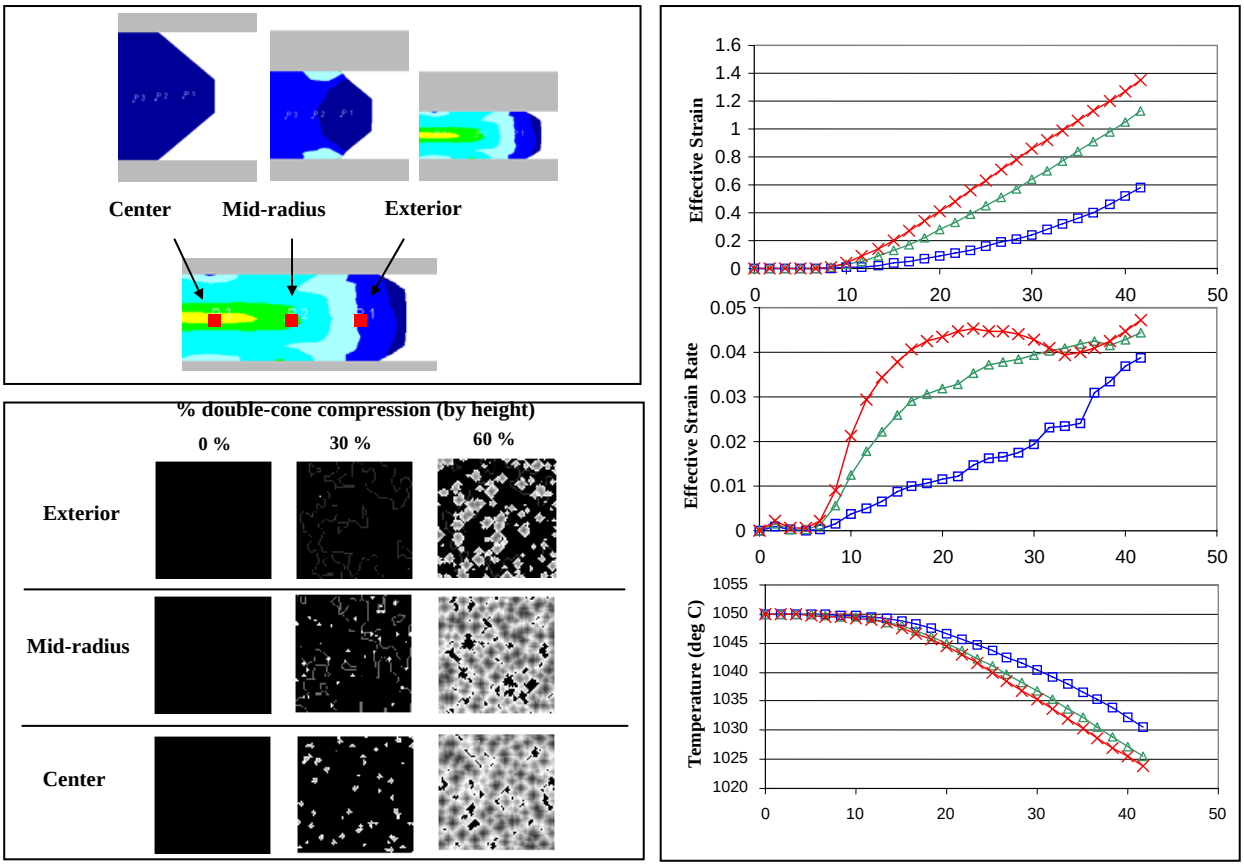


Figure 6. Methodology for Discrete Lattice Modeling. ***(Top left)*** **An FEM simulation is performed, and regions of interest are "point-tracked": strain, strain rate, temperature histories are interpolated at those points.** ***(Right)*** **The strain, strain rate, and temperature histories of the regions of interest.** ***(Bottom left)*** **The predicted simulated recrystallization regions of the Discrete Lattice model, at three different points within a double-cone compression test (exterior, mid-radius, and center), displayed at three different degrees of compression of the double-cone test specimen (0%, 30%, and 60%). Dark regions represent non-recrystallized material; lighter regions represent recrystallized material. Discrete Lattice model (bottom graph).**

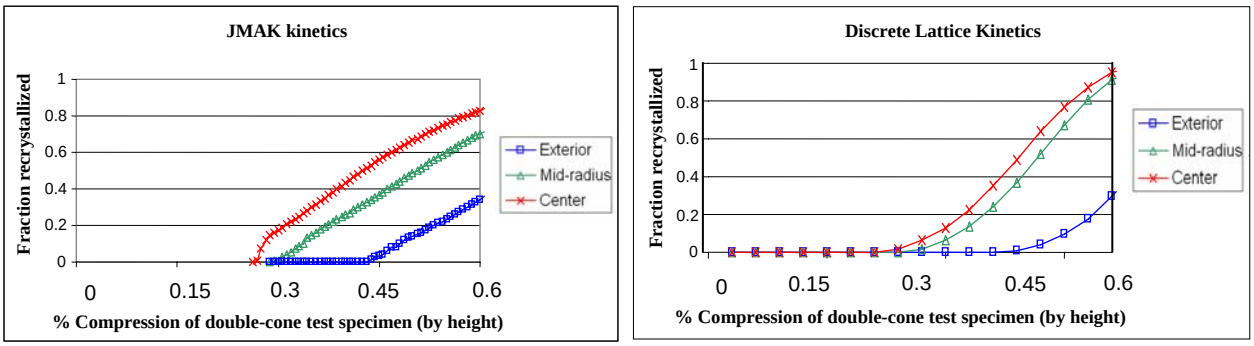


Figure 7. Comparison of kinetics of dynamic recrystallization as predicted by classical JMAK modeling (left) vs. Discrete Lattice modeling (right). The fraction recrystallized is plotted as a function of compression of the double-cone test specimen for each region of interest tracked in Figure 7.

Figure 8 displays an example of two different initial microstructures with nearly identical grain size distribution statistics but with very different grain shapes. Each has an equivalent grain area, but the "equiaxed" microstructure has roughly isotropically shaped grains, and the "elongated" microstructure consists of non-equiaxed grains. Since classical JMAK modeling generally only receives and determines the "average" grain size as a description of the microstructure morphology, the kinetics of recrystallization predicted by JMAK would be the same for both example microstructures. Each was exposed to the same thermomechanical history predicted by point-tracking a region of a compressing cylinder, and each modeled the same microstructural phenomena parameters with the same materials constants values. However, as exhibited in the graph below, the kinetics modeled via Discrete Lattice microstructure evolution are in fact different (due to extra grain boundary surface area and hence higher nucleation rates, and narrower grain thicknesses and hence faster impingement of recrystallizing grains). At around 0.75 strain, the "equiaxed" microstructure is 59% recrystallized, whereas the microstructure with elongated grains is 68% recrystallized at the same degree of deformation. This represents approximately a 15% difference. Taking into consideration that the dislocation density of recrystallized vs. unrecrystallized material can be several orders of magnitude lower, and that flow stress is a strong function of dislocation density, this small fraction can significantly affect the final properties. (Note: repeated modeling of the same TMP histories on different microstructures result in much subtler, statistically insignificant

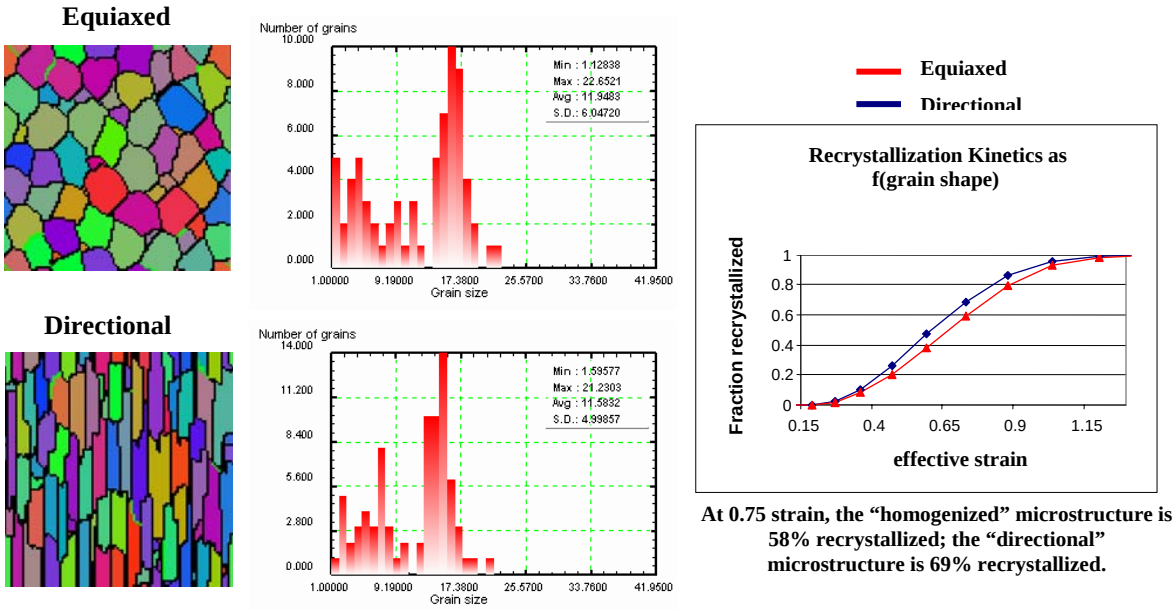
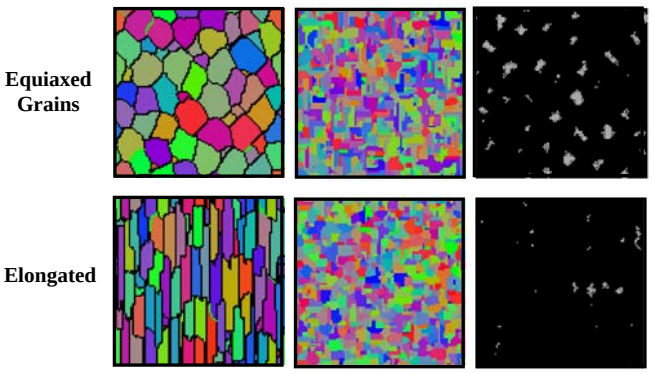


Figure 8. Demonstration of the sensitivity of Discrete Lattice modeling to different initial microstructure morphologies. (Left) two microstructures with different grain morphologies yet equivalent average grain sizes; (center) nearly-equivalent grain size distributions of each microstructure; (right) different resultant kinetics of recrystallization as a function of the different grain shapes.

differences in kinetics). Furthermore, if one is concerned about occasional large grains present in the microstructure (as are many materials suppliers, who may guarantee outgoing material specifications), the difference between the two models is more conspicuous, as observed in Figure 9.

Figure 9. *(Left)* Two different initial microstructures – equiaxed grains and elongated grains – exposed to the same thermomechanical history and with the same microstructure evolution parameters. *(Center)* Final microstructures after dynamic recrystallization and grain growth. *(Right)* Unrecrystallized grains (grey regions) are significantly different.



Discrete Lattice Modeling –Ingot Breakdown of Non-Uniform Microstructure

Discrete Lattice modeling kinetics have thus been shown to compare favorably with the tried-and-true kinetics predictions of classical JMAK modeling. It was further shown that Discrete Lattice modeling is sensitive to real-world microstructure issues such as non-equiaxed initial grain shapes. Hence, it is now possible to run a simulation with multiple different starting microstructures within a workpiece, and to observe the effect of different processing parameters on the resultant, final microstructure. In this manner, it is possible to design and simulate a thermo-mechanical process to optimally homogenize the initially highly non-uniform grains across a cast ingot into a finer-grained, uniform microstructure. The example process given below (Figure 10) is the cogging of a large-grained, cast ingot.

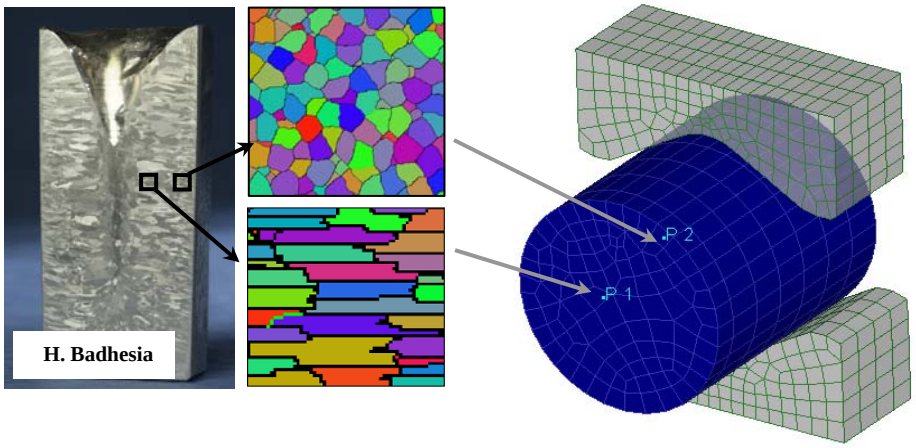


Figure 10. ***(Left)*** **Large-grained cast ingot with a varying microstructure (*Courtesy H. K. D. H. Badhesia, Univ. of Cambridge*[7]). *(Center)* Example microstructures with similar grain sizes and shapes. *(Right)* Location of material point-tracked in a cogged workpiece. The thermo-mechanical histories from these points will be provided as inputs to the Discrete Lattice model for each simulated microstructure.**

During the cogging process, the ingot is heated to working temperature, at which point grain growth can occur. Dies make several passes along the ingot – as they pass along the point-tracked regions, they induce work hardening (strain) in the simulated microstructures of Figure 10. When a critical strain is reached, the material may recrystallize, resulting in a decrease in average grain size (Figure 11). In between passes of the dies, which may last from a few seconds to a few minutes, the material may continue to experience metadynamic or static recrystallization and grain growth, which results in an increase in the average grain size. Since this process of recrystallization and grain growth may experience one or more cycles during the cogging process, the final grain size across the ingot, regardless of the initial grain sizes, will begin to become more uniform. This uniformity may be measured at the end of the process, and quantified in terms of the cogging parameters. In this manner the cogging parameters may be tweaked until a desired microstructural result is reached. The strain rate vs. time of each tracked point in this example cogging simulation, as well as the average grain size vs. time of each tracked point, are presented in Figure 11.

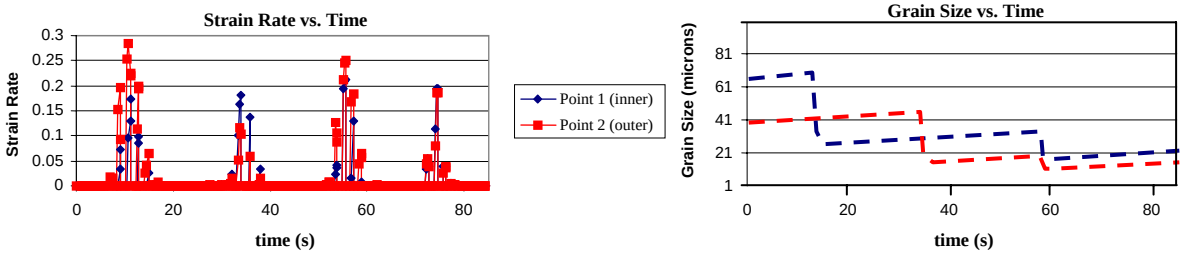


Figure 11. ***(Top)*** **Graph of strain rate vs. time for the two regions point-tracked in the cogged ingot of Figure 10. *(Bottom)* Graph of average grain size for the two microstructures representing the material at the points tracked. When a critical strain is reached during a pass of the dies, the material recrystallizes, resulting in a finer grain size. In between passes of the dies, the material experiences grain growth, and the grains increase in size.**

Summary and Future Work

A new Cellular Automata (CA) microstructure model has been developed and integrated into the commercial FEM code DEFORM^{TM}. This model can generate statistically realistic initial microstructures from a starting initial grain size, and currently quantifies microstructural phenomena such as work hardening, recovery, dynamic recrystallization, metadynamic recrystallization, static recrystallization, and grain growth, as functions of thermomechanical inputs strain, strain rate, and temperature, and of microstructural parameters such as crystallographic orientation, grain boundary misorientation, and dislocation density.

The kinetics of the model compare well qualitatively and quantitatively to classical JMAK model kinetics. Additionally, the new CA model can capture differences in kinetics due to varying grain shape – something which JMAK modeling is typically insensitive to. This permits the optimization of processes such as ingot conversion during cogging, whereby initially non-uniform grains are refined to a uniform microstructure in an efficient manner.

Future development includes modeling precipitation and phase transformation, as well as microstructure initialization from a grain size distribution (rather than simply an average grain size), a micrograph, or an Electron Backscatter Diffraction (EBSD) file. An Inverse Analysis technique to back-calculate unknown materials constants from known experimental data (such as flow stress or recrystallization curves) will also be developed. The microstructure evolution model as well as the Inverse Analysis technique will be validated with laboratory and industrial scale experiments of U720 over the course of second phase of this project.

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